Monthly report for March, 2007

In the last month, I have been working on the following proposed by Dr. Rivers and his colleagues.

1. Completed in the last month.

(1). **Q**: Be compatible for different kind of raw data files, like .mar3450, .tiff etc.

A: Now the CEAD can automatically deal with the .mar3450 and tif files.

(2). **Q**: In case of tens or hundreds of input files, how to easily input the raw data files.

A: Assume that inputting the pressure/temperature values manually is unnecessary.

A new task was developed for this purpose (shown in figure 1). It requires inputting

the first file, last file, and the file base etc, as long as the files # less than 9999.
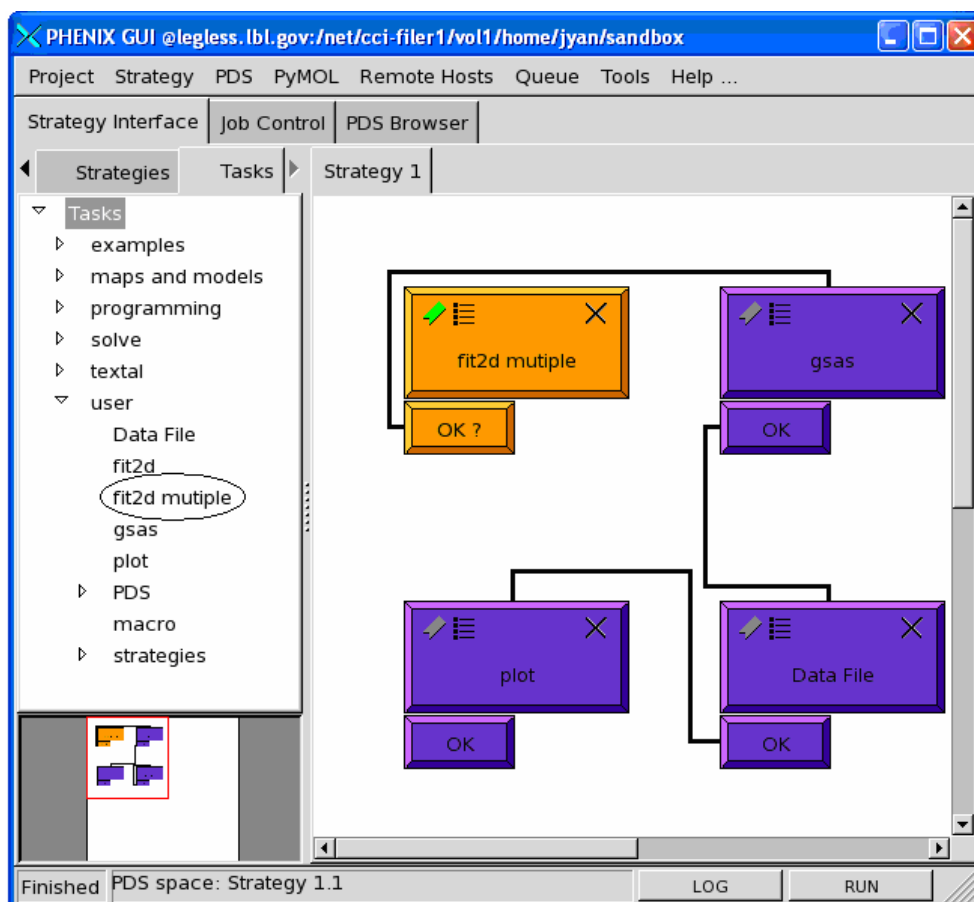

Figure 1. A task (fited multiple) developed for tens or hundreds of raw data files.

Figure 2. The input window fit2d multiple task

√ (3). **Q**: Add a pixel size input box, mask threshold setting and data limit of the 1-D in CEAD.

A: These features have been added to the CEAD shown in figure 2.

√ (4). **Q**: Add Error bar in the plot

A: This feature has been added to the CEAD. Users can choose to display the unit cell volume or lattice constant, with either error bar or no error bar.
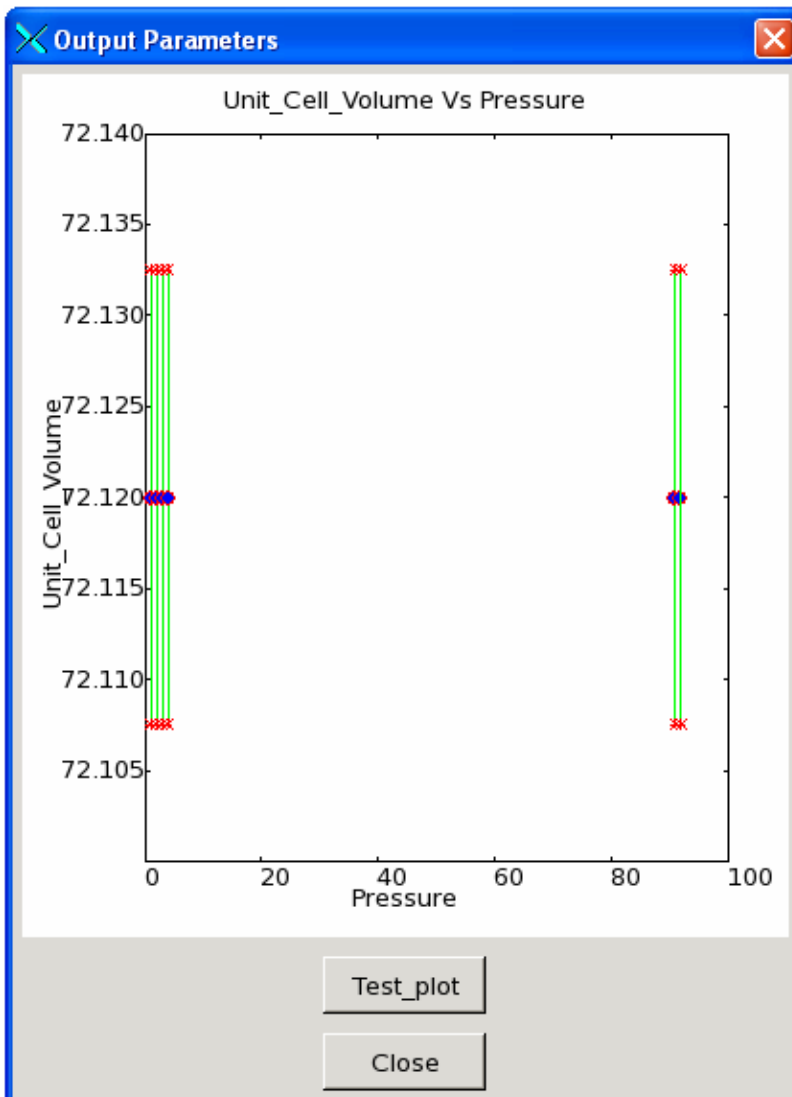
plot Input Parameters

[Save]   [Close]

UNIT CELL VOLUME / LATTICE CONSTANT?

VOLUME/LATTICE_CONST

CHOICE   [VOLUME   ◆]   Please select:
                              ERROR_BAR   ◆
                              NO_ERROR_BAR

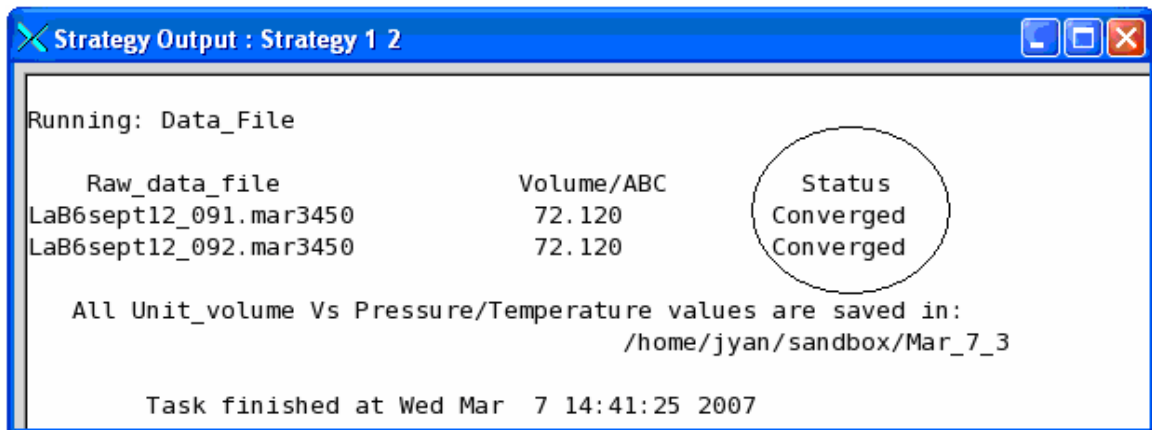## Output Parameters

Unit_Cell_Volume Vs Pressure

√ (5). **Q**: Add a warning prompt or window

A: In the log file, warning messages are listed at the "status" column after each run.

"Converged" displayed if "Convergence was achieved" in .LST file

"Diverging" displayed if "System equation is diverging" in .LST file

Otherwise, "Not Converged" will be displayed

2. To be completed the next.

(1). Add a mask file calling function

Up to now, I could not find where to add it in fit2d. I have not received response

from Andy Hammersley yet.

(2). Space group information input [manually input/CIF file]

(3) Double phase refinement in gsas.

(4) The iteration of the unit cell values from the last round.